THU-94-12
comp-gas/9501001

Algebraic Spatial Correlations and Non-Gibbsian Equilibrium States[1]

M.H. Ernst and H.J. Bussemaker

Institute for Theoretical Physics
University of Utrecht
Princetonplein 5, P.O.Box 80.006
3508 TA Utrecht, The Netherlands

Abstract

Non-Gibbsian stationary states occur in dissipative non-equilibrium systems. They are closely connected with the lack of detailed balance and the absence of a fluctuation-dissipation theorem. These states exhibit spatial correlations that are long ranged under generic conditions, even in systems with short range interactions, provided the system has slow modes and some degree of spatial anisotropy. In this paper we present a theory for static pair correlations in lattice gas automata violating detailed balance, and we show that the spatially uniform non-Gibbsian equilibrium state exhibits long range correlations, even in the absence of an external driving field.

Key words: long rang spatial correlations, violation of detailed balance, fluctuation-dissipation theorem, lattice gas automata.

[1] contribution to Princeton meeting 'Discrete Models for Fluid Dynamics,' held June 27-29, 1994

1 Introduction

As highlighted in a recent review by Dorfman et al. [1], a major theme in non-equilibrium statistical mechanics during the past few decades has been the question under what conditions the correlations in fluids, that consist of molecules with short-range interactions, can become long-ranged. The existence of generic long range spatial correlations in non-equilibrium stationary states of condensed matter (e.g. systems with a constant temperature gradient, driven diffusive systems [2]) is by now well understood, and is intimately connected with the existence of long time tails in Green-Kubo type time correlation functions. In this paper we discuss the occurrence of such correlations in lattice gas automata (LGA's).

The long range correlations can be described at three different levels of microscopic detail: (i) The macroscopic phenomenological equation (diffusion, Navier-Stokes) with a Langevin noise term added [3, 4]. Here the transport coefficients and noise strengths are phenomenological input in the theory. A summary of this approach will be given in section 2. (ii) The kinetic (Boltzmann) equation to which a Langevin noise term is added [5]. Here the transport coefficients are determined by the theory, but the noise strength is phenomenological input. This intermediate level of description will not be pursued here. For applications to LGA's we refer to Ref. [6]. (iii) A fully microscopic statistical mechanical description. Here both the noise strength and the transport coefficient are calculated from the theory.

To obtain a description at the fully microscopic level, one starts from the equations of motion for the dynamic variables or the phase space density, and then derives a BBGKY-hierarchy for the distribution functions. After appropriate approximations one obtains kinetic equations for the single particle and pair correlation functions. Long range spatial and temporal correlations are created by sequences of ring collisions.

If a classical fluid is in thermodynamic equilibrium, long range spatial correlations only occur under very special conditions, when parameters like the temperature are tuned to a critical value. In general however the correlation length is finite. The situation is different when external driving fields or constraints imposed by external reservoirs prevent the fluid from achieving a thermodynamic equilibrium state satisfing the constraints of detailed balance. In this case *generic* long range spatial correlations exist in the non-equilibrium stationary state, for almost all parameter values.

The same concepts are also directly relevant for LGA's that violate the constraints of (semi)-detailed balance. Recently, a microscopic theory at the level of pair correlations (ring kinetic theory) has been applied to LGA's to calculate the equal-time position and velocity correlations in spatially uniform equilibrium states [7]. The primary goal of the present paper is to apply the ring kinetic theory to demonstrate the existence of generic long range spatial correlations in uniform equilibria of LGA's without detailed balance. This will be worked out in section 3. The coarsest description, by means of a fluctuationg diffusion equation, is conceptually the simplest, but it captures all essential features. It will be discussed in section 2.

All three levels of description share the same essential ingredients for the existence of such algebraic correlations: (i) the existence of local conservation laws or slow (diffusive or hydrodynamic) modes; (ii) lack of detailed balance; (iii) some degree of anisotropy, either due to the underlying lattice, or due to an external driving field or gradient imposed by external reservoirs.

2 Langevin Equation

A clear presentation of the basic theory of non-equilibrium Langevin models has been given by Grinstein et al. [3, 4]. Here we only indicate the essential steps. Consider a locally conserved density $h(\boldsymbol{r},t) = \langle \hat{h}(\boldsymbol{r},t) \rangle$. On average it satisfies a diffusion equation with an anisotropic diffusion tensor. To account for the fluctuations, a Langevin noise term is added to this equation. It reads after Fourier transformation,

$$\partial_t \hat{h}(\boldsymbol{q},t) = (D_x q_x^2 + D_y q_y^2)\hat{h}(\boldsymbol{q},t) + \hat{\eta}(\boldsymbol{q},t), \tag{2.1}$$

where the Gaussian random noise is determined by

$$\langle \hat{\eta}(\boldsymbol{q},t)\hat{\eta}(-\boldsymbol{q},t') \rangle = 2(B_x q_x^2 + B_y q_y^2)\delta(t-t'). \tag{2.2}$$

We allow for spatial anisotropy by having two constants B_x and B_y. The diffusion coefficients D_α and noise strengths B_α are phenomenological coefficients; they are not provided by the theory. Without loss of generality we use a two-dimensional presentation to denote longitudinal and transverse directions with respect to the wave vector $\boldsymbol{q}$.

The equal time density-density correlation function in the stationary state, $G(\boldsymbol{r},\infty) \equiv \mathcal{G}(\boldsymbol{r})$, is given by

$$\mathcal{G}(\boldsymbol{r}) = \int \frac{d\boldsymbol{q}}{(2\pi)^d} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \chi(\boldsymbol{q}). \tag{2.3}$$

Here d is the number of dimensions and the stationary susceptibility can be calculated from (2.1) and (2.2) as,

$$\chi(\boldsymbol{q}) = \lim_{t\to\infty} \langle |\hat{h}(\boldsymbol{q},t)|^2 \rangle = \frac{B(\boldsymbol{q})}{D(\boldsymbol{q})} = \frac{B_x \hat{q}_x^2 + B_y \hat{q}_y^2}{D_x \hat{q}_x^2 + D_y \hat{q}_y^2}, \tag{2.4}$$

where $\hat{q}_\alpha = q_\alpha/|\boldsymbol{q}|$ is a Cartesian component of a unit vector ($\alpha = x, y, \ldots, d$).

Possible scenario's:

(i) If the system satisfies *detailed balance*, i.e. if the equilibrium distribution is given by the Gibbs distribution, the equilibrium value of the susceptibility $\chi(\boldsymbol{q}) \simeq \chi_0$ as $q \to 0$ is known from thermodynamics, and transport coefficients and noise strengths are related by the *fluctuation-dissipation* theorem, $B(\boldsymbol{q}) = \chi_0 D(\boldsymbol{q})$. The correlation function is short-ranged, $G(\boldsymbol{r}) \simeq \chi_0 \delta(\boldsymbol{r})$.

(ii) However *without* the detailed balance constraint, the equilibrium state is not a thermodynamic state, and the corresponding susceptibilities are unknown. There is *no* fluctuation-dissipation theorem imposing a relationship between $B(\boldsymbol{q})$ and $D(\boldsymbol{q})$. The long wavelength limit $\chi_0(\hat{q})$ of the susceptibility is in general *anisotropic* and depends on the direction of $\hat{q}$. A rescaling of the integration variables in (2.3), namely $\boldsymbol{q} = \boldsymbol{k}/r$, shows that $G(\boldsymbol{r}) \sim r^{-d}$ at large distances. As diffusive modes are correlated over time intervals $t \sim r^2$, the spatial correlations $\sim r^{-d}$ have an intimate connection with the long time tails $t^{-d/2}$ in the velocity and other current-current correlation functions [8]. For later reference we quote the explicit form of the correlation function (2.3) at large distances in two dimensions, where the susceptibility is given by (2.4), i.e.

$$G(\boldsymbol{r}) = G(x,y) \simeq \frac{1}{\pi\sqrt{D_x D_y}} \left(\frac{D_x B_y - D_y B_x}{D_y x^2 + D_x y^2} \right). \tag{2.5}$$

As we shall see in section 3, this scenario is realized in LGA's where the collision rules do not satisfy detailed balance *and* break the lattice symmetry by having different transition probabilities in x- and y-direction.

(iii) Different scenario's are realized when the phenomenological $B(\boldsymbol{q})$ and/or $D(\boldsymbol{q})$, and therefore also $\chi(\boldsymbol{q})$ in (2.4), have a weaker anisotropy as $q \to 0$, that only shows up in terms of relative order $\mathcal{O}(q^2)$ or $\mathcal{O}(q^4)$. Then $G(\boldsymbol{r})$ decays again algebraically on account of (2.3), with a tail proportional to $1/r^{d+2}$ or $1/r^{d+4}$ respectively.

Suppose that one wants to describe a system where the microscopic transition probabilities have the symmetry of a d-dimensional lattice, but where there is *no* externally imposed direction in which the *lattice symmetry is broken*. Examples are the spin-spin correlations on hypercubic lattices as discussed by Grinstein [4], or several non-detailed balance LGA's on square, triangular, or FCHC lattices (see sections 3 and 4).

The general form of the noise strength for small q is

$$q^2 B(\boldsymbol{q}) = q_\alpha q_\beta B_{\alpha\beta} + q_\alpha q_\beta q_\gamma q_\delta B^4_{\alpha\beta\gamma\delta} + \mathcal{O}(q^6), \tag{2.6}$$

and a similar expansion holds for the transport coefficient $q^2 D(\boldsymbol{q})$. Greek indices denote Cartesian components and summation convention is used for repeated indices. The coefficients $B_{\alpha\beta}, D_{\alpha\beta}$ and $B^4_{\alpha\beta\gamma\delta}, D^4_{\alpha\beta\gamma\delta}$ are respectively tensors of rank 2 and rank 4. On all lattices with 4- or 6-fold symmetry, the second rank tensors are *isotropic*, i.e. $B_{\alpha\beta} = B\delta_{\alpha\beta}$.

Fourth rank tensors $\boldsymbol{B}^4$ and $\boldsymbol{D}^4$ are only *isotropic* on the two-dimensional triangular lattice and the four-dimensional FCHC lattice, and *anisotropic* on all other lattices in two and three dimensions. In the latter cases the susceptibility for $q \to 0$ behaves as $\chi(\boldsymbol{q}) = \chi_0 + q^2\chi_2(\hat{q})$ and $G(\boldsymbol{r}) \sim 1/r^{d+2}$. In the former cases the susceptibility has the form $\chi(\boldsymbol{q}) = \chi_0 + q^2\chi_2 + q^4\chi_4(\hat{q})$ and $G(\boldsymbol{r}) \sim 1/r^{d+4}$. For later reference we calculate the results for a square lattice. There $\chi_2(\hat{q}) = E_s + E_a\left(\hat{q}_x^4 + \hat{q}_y^4\right)$, and $G(\boldsymbol{r})$ in (2.3) approaches

$$G(\boldsymbol{r}) \simeq -6E_a/\pi r^4 \qquad (r \to \infty). \tag{2.7}$$

In the microscopic LGA's violating detailed balance, to be discussed in section 3 and 4, the coefficients $B(\boldsymbol{q})$ and $D(\boldsymbol{q})$ can be calculated explicitly from the ring kinetic theory, and yield the coefficients of the algebraic tails in $G(\boldsymbol{r})$.

3 Ring Equation for LGA's

In this section we present the ring kinetic theory for velocity and spatial correlations in LGA's violating detailed balance with respect to the Gibbs distribution. Such correlations have been observed in several models by various authors [9, 10, 11].

Starting from a BBGKY hierarchy for the n-particle distribution functions, we use cluster expansion techniques to derive approximate kinetic equations. In zeroth approximation the standard nonlinear Boltzmann equation is obtained; the next approximation yields the ring kinetic equation, similar to that for hard sphere systems, describing the time evolution of pair correlations. The derivation of the generalized Boltzmann equation and ring equation can be found in Ref. [7]. Here we only sketch the results in so far as they are needed for the present analysis. Similar cluster expansion techniques have been developed in Ref. [12].

The collision step of a LGA is defined by the strictly local transition probabilities $A_{s\sigma}$ from a precollision state s at a single node to a postcollision state σ at the same node. It is followed by a propagation step.

Much is known about LGA's that satisfy the condition of semi-detailed balance, $\sum_s A_{s\sigma} = 1$, or (stronger) detailed balance, $A_{s\sigma} = A_{\sigma s}$, with respect to the Gibbs distribution. The equilibrium Gibbs distribution depends only on the globally conserved quantities, such as the total number of particles N, the total momentum P or the total energy E. The Gibbs distribution is completely factorized: no equal-time correlations between occupation numbers exist.

In LGA's without detailed balance $\sum_s A_{s\sigma} \neq 1$. Starting from a completely factorized precollision state, the collisions will then create postcollision correlations between occupation numbers at the same node. The postcollision on-node correlation for $i \neq j$ are given by [7, 11]

$$\langle \sigma_i \sigma_j \rangle^* \equiv \sum_{s\sigma} \sigma_i \sigma_j A_{s\sigma} F(s) \neq f_i f_j, \tag{3.1}$$

where we have introduced the average occupation number $f_i = \langle s_i \rangle$. The completely factorized distribution function $F(s)$ is given by

$$F(s) = \prod_i f_i^{s_i} (1 - f_i)^{1-s_i}. \tag{3.2}$$

Due to subsequent propagation and collision steps the postcollision on-node correlations will be transformed into on- and off-node precollision correlations, via a process of scattering by other particles in the system (ring collisions).

If we neglect all correlations between occupation numbers, the time evolution of the one-particle distribution function, $f_i(\mathbf{r}, t) = \langle s_i(\boldsymbol{r}, t)\rangle$, is given by the nonlinear Boltzmann equation [6],

$$f_i(\boldsymbol{r} + \boldsymbol{c}_i, t+1) = f_i(\boldsymbol{r}, t) + \Omega_i(f(\boldsymbol{r}, t)), \tag{3.3}$$

where $\boldsymbol{r}$ labels the nodes and $\boldsymbol{c}_i$ the nearest neighbor links. For the detailed definition of $\Omega_i(f)$ in terms of $A_{s\sigma}$ we refer to Ref. [7]. At a more refined level of description we include all pair correlations between fluctuations ($\delta s_i = s_i - f_i$),

$$G_{ij}(\boldsymbol{r}, \boldsymbol{r}', t) \equiv \langle \delta s_i(\boldsymbol{r}, t) \delta s_j(\boldsymbol{r}', t)\rangle. \tag{3.4}$$

The coupled time evolution of $f_i(\boldsymbol{r}, t)$ and $G_{ij}(\boldsymbol{r}, \boldsymbol{r}', t)$ is then given by the *generalized* Boltzmann equation

$$f_i(\boldsymbol{r} + \boldsymbol{c}_i, t+1) = f_i(\boldsymbol{r}, t) + \Omega_i(f(\boldsymbol{r}, t)) + \sum_{k<\ell} \Omega_{i,k\ell}(f(\boldsymbol{r}, t)) G_{k\ell}(\boldsymbol{r}, \boldsymbol{r}, t), \tag{3.5}$$

together with the *ring* kinetic equation

$$G_{ij}(\boldsymbol{r} + \boldsymbol{c}_i, \boldsymbol{r}' + \boldsymbol{c}_j, t+1) = \delta(\boldsymbol{r}, \boldsymbol{r}') B_{ij}(\boldsymbol{r}, t) + \sum_{k,\ell} \omega_{ij,k\ell} G_{k\ell}(\boldsymbol{r}, \boldsymbol{r}', t). \tag{3.6}$$

Here the linear pair collision operator is given by

$$\omega_{ij,k\ell} = \{\delta_{ik} + \Omega_{ik}(f(\boldsymbol{r}, t))\}\{\delta_{j\ell} + \Omega_{j\ell}(f(\boldsymbol{r}, t))\}. \tag{3.7}$$

In the equations above we have introduced $\Omega_{ik} = \partial\Omega_i/\partial f_k$ and $\Omega_{i,k\ell} = \partial^2\Omega_i/\partial f_k \partial f_\ell$. The on-node source term $B_{ij}(\boldsymbol{r}, t)$ depends on $f_j(\boldsymbol{r}, t)$ and $G_{ij}(\boldsymbol{r}, \boldsymbol{r}, t)$, and essentially represents the correlations created by the collision step.

The explicit form of the matrix elements Ω are not needed in the present analysis, where we focus on the large-$\boldsymbol{r}$ behavior of the solution of (3.6) in the uniform equilibrium state. The on-node source term contains a dominant contribution, referred to as the simple ring approximation, which will be given below for the special case of equilibrium. Here we neglect subleading terms,

linear in the pair correlation function [7], which correspond to the 'repeated ring approximation' in the theory of continuous fluids.

A spatially homogeneous equilibrium solution obeys the relation $f_i(\boldsymbol{r},\infty) = f_i$ and $G_{ij}(\boldsymbol{r},\boldsymbol{r}',\infty) = \mathcal{G}_{ij}(\boldsymbol{r}-\boldsymbol{r}')$. For a given average occupation f_i, the correlations can be obtained from a linear equation,

$$\mathcal{G}_{ij}(\boldsymbol{r}) = v_0 \int_{1\mathrm{BZ}} \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^d} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \left[\frac{1}{1-s(\boldsymbol{q})\omega} s(\boldsymbol{q}) B\right]_{ij}, \tag{3.8}$$

with v_0 the volume of the unit cell of the direct lattice ($v_0 = 1$ for square and cubic lattices and $v_0 = \frac{1}{2}\sqrt{3}$ for triangular lattices), and the pair streaming operator given by

$$s_{ij}(\boldsymbol{q}) = \exp[i\boldsymbol{q}\cdot(\boldsymbol{c}_j - \boldsymbol{c}_i)]. \tag{3.9}$$

The on-node source term

$$B_{ij} = B_{ij}(\boldsymbol{r},\infty) = \langle\sigma_i\sigma_j\rangle^* - \langle s_i s_j\rangle \tag{3.10}$$

equals the change in on-node correlations caused by the collision step in equilibrium, where $\langle\ldots\rangle^*$ is defined in (3.1) ($B_{ij} = 0$ in SDB-models).

The spatial correlation functions of most interest are those between conserved densities, defined as

$$\mathcal{G}_{ab}(\boldsymbol{r}) = \sum_{ij} a_i b_i \mathcal{G}_{ij}(\boldsymbol{r}) \equiv \langle ab|\mathcal{G}(\boldsymbol{r})\rangle, \tag{3.11}$$

where a_i and b_i are collisional invariants. In a purely diffusive system $a_i = b_i = 1$, in a thermal fluid-type LGA $a_i, b_i = \{1, c_{\alpha i}, \frac{1}{2}c_i^2\}$. Moreover, we note the important conservation law $\langle ab|B\rangle = 0$ as implied by (3.10), stating that the source term B is orthogonal to products of collisional invariants.

The numerical calculation of $\mathcal{G}_{ij}(\boldsymbol{0})$ for given f_i involves matrix inversion and integration over the first Brillouin zone. Since f_i again depends on $\mathcal{G}_{ij}(\boldsymbol{0})$, we use an iterative scheme to find a self-consistent solution $\{f_i, \mathcal{G}_{ij}(\boldsymbol{0})\}$. Once $\mathcal{G}_{ij}(\boldsymbol{0})$ is known, all off-node correlations $\mathcal{G}_{ij}(\boldsymbol{r})$ can be calculated from it in a straightforward way. For details we refer to Ref. [7].

The analytical calculation of (3.8) can be carried through for large spatial distances ($r \to \infty$) or small wave numbers ($q \to 0$). The essential observation is that the *pair* operator $s(\boldsymbol{q})\omega$ in (3.8) has *slow* (diffusive) modes $\chi_{\mu\nu}(\boldsymbol{q})$ with eigenvalues behaving like $\Lambda_{\mu\nu}(\boldsymbol{q}) \simeq 1 - q^2 D_{\mu\nu}(\hat{q}) + \ldots$ for small q, where

$D_{\mu\nu}(\hat{q})$ may depend on the direction of $\boldsymbol{q}$. The slow modes give rise to singular denominators in (3.8), and are responsible for the large-$\boldsymbol{r}$ behavior of $\mathcal{G}_{ab}(\boldsymbol{r})$.

To analyze this more systematically it is convenient to make a spectral decomposition of the pair operator $s(\boldsymbol{q})\omega$ in (3.8), i.e.

$$\mathcal{G}_{ab}(\boldsymbol{r}) \simeq v_0 {\sum_{\mu\nu}}^* \int_{1BZ} \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^d} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \frac{\langle ab|\chi_{\mu\nu}(\boldsymbol{q})\rangle\langle\tilde{\chi}_{\mu\nu}(\boldsymbol{q})s(\boldsymbol{q})|B\rangle}{1-\Lambda_{\mu\nu}(\boldsymbol{q})}. \tag{3.12}$$

Here $\chi_{\mu\nu}$ and $\tilde{\chi}_{\mu\nu}$ are respectively right and left eigenfunctions (product modes) of the pair operator $s(\boldsymbol{q})\omega$ with eigenvalue $\Lambda_{\mu\nu}(\boldsymbol{q})$. These product modes form a complete bi-orthogonal set of basis functions in the pair space, i.e. $\langle\tilde{\chi}_{\mu\nu}|\chi_{\mu'\nu'}\rangle = \delta_{\mu\mu'}\delta_{\nu\nu'}$. The asterisk in (3.12) indicates that the $\mu\nu$-summation is restricted to pairs of slow (hydrodynamic or diffusive) modes.

To make these results more explicit we specialize to a purely diffusive model on a square lattice. Here $a_i = b_i = 1$ are the only collisional invariants, and the only slow pair mode $\chi_{DD}(\boldsymbol{q})$ is a product of single particle diffusive modes. The conservation laws imply $\langle 11|B\rangle = 0$, and the lattice symmetry guarantee that $\langle\tilde{\chi}_{DD}(\boldsymbol{q})s(\boldsymbol{q})|B\rangle = q^2 B(\boldsymbol{q})$ where $B(\boldsymbol{q})$ has the general form (2.6). The denominator, $1-\Lambda_{DD}(\boldsymbol{q}) = 2q^2 D(\boldsymbol{q})$, has a similar form for small q. Moreover, one can show that $\langle 11|\chi_{DD}\rangle = 1+\mathcal{O}(q^2)$. The (non)-isotropy of the second and fourth rank tensors $\boldsymbol{B}, \boldsymbol{D}$ and $\boldsymbol{B}^4, \boldsymbol{D}^4$ respectively, depends on the microscopic collision rules of the lattice model under consideration.

In *summary*, we have established that the spatial correlation functions $\mathcal{G}_{ab}(\boldsymbol{r})$ in equilibrium approach for large r the generic form (2.3) and (2.4) of the phenomenological theory of section 2, and in addition we have provided expressions for the tensors $\boldsymbol{B}, \boldsymbol{D}$ and $\boldsymbol{B}^4, \boldsymbol{D}^4$, leading to a complete microscopic theory for long range behavior of the spatial correlation functions of LGA's violating the detailed balance constraints.

4 Interacting Random Walkers

4.1 Spatial Symmetry

To illustrate the general results of the previous sections we first consider a model of interacting random walkers on a square lattice with Fermi exclusion. There is no breaking of the lattice symmetry in the microscopic transition probabilities. The model allows for at most *one* particle per state $\{\boldsymbol{r}, \boldsymbol{c}_i\}$

(i = 1,2,3,4) where $\boldsymbol{r}$ labels a lattice node and $\boldsymbol{c}_i$ a nearest neighbor link. The in-state or pre-transition state of the node is described by the set of occupation numbers $s(\boldsymbol{r}) = \{s_i(\boldsymbol{r}); i = 1, 2, 3, 4\}$, and similarly the out-state or post-transition state is described by $\sigma(\boldsymbol{r}) = \{\sigma_i(\boldsymbol{r}); i = 1, 2, 3, 4\}$. The dynamics consists of local transitions, followed by propagation. The local transitions conserve the number of particles.

If there is only *one* particle at node $\boldsymbol{r}$, it behaves like a random walker; if there are *three* particles at $\boldsymbol{r}$, or equivalently one hole, the hole behaves like a random walker. If there are *no* particles or no holes, in- and out-states are identical. To describe the *two*-particle interactions, let $\{ij\}$ denote the two-particle state in which links i and j are occupied. Then the transitions are defined as,

$$\{13\}, \{24\} \underset{\beta}{\overset{\alpha}{\rightleftarrows}} \{12\}, \{23\}, \{34\}, \{41\} \tag{4.1}$$

where α denotes the transition probability of any state on the left to any on the right, and β the probability for the reverse transition. We note that the states on the right, and those on the left of (4.1) are not connected by lattice symmetries. If we denote the transition probabilities among the four states on the right hand side by γ, and those among the ones on the left by δ, then we have the normalization conditions $4\alpha + 2\delta = 1$ and $2\beta + 4\gamma = 1$.

In case $\alpha \neq \beta$ the matrix of transition rates, $A_{s\sigma} \neq A_{\sigma s}$, does not obey the (semi)-detailed balance conditions of section 3. The transitions in (4.1) create correlations between different velocity links, and the pre-transition correlations $\langle s_i s_j \rangle$ differ from the post-transition ones $\langle \sigma_i \sigma_j \rangle^*$ in (3.10), even in the uniform equilibrium state. Consequently, B_{ij} in (3.10) is nonvanishing, and so is $q^2 B(\boldsymbol{q})$ in (2.6). Because of the square symmetry the second rank tensor $B_{\alpha\beta} = B\delta_{\alpha\beta}$ in (2.6) is isotropic, but the fourth rank tensor $B^4_{\alpha\beta\gamma\delta}$ is not, which leads immediately to the $1/r^4$ tail in (2.7). The coefficient E_a is proportional to $(\alpha - \beta) f^2 (1 - f)^2$ where $f = \frac{1}{4}\rho$ is the reduced average density.

In case $\alpha = \beta$ the *detailed balance* constraints are satisfied, and the transitions do *not* create any correlations in the stationary state, i.e. $\langle \sigma_i \sigma_j \rangle^* = \langle s_i s_j \rangle = f_i f_j$, and long range correlations are absent. The details of these calculations and the explicit value of the coefficient E_a of the algebraic tail will be given elsewhere [13].

4.2 Broken Spatial Symmetry

The long range correlations will be much stronger if the microscopic transition probabilities are anisotropic. It is a driven diffusive system that remains spatially uniform in the stationary state. For purpose of illustration we consider again a diffusive 4-bit LGA on a square lattice where the local transition probabilities in x- and y-directions are different, i.e.

$$A_{s\sigma} = \frac{1}{Z(s)}\delta(\rho(s), \rho(\sigma)) \exp[b j_x(s) j_x(\sigma)]. \tag{4.2}$$

Here $j_x(s) = \sum_i c_{xi} s_i(r)$ represent the local particle current in the $\hat{x}$-direction. The local number of particles $\rho(s) = \sum_i s_i(r)$ in the in-state, as well as $\rho(\sigma)$ in the out-state is conserved, and $Z(s)$ is a normalization constant chosen such that $\sum_\sigma A_{s\sigma} = 1$. For positive b-values transitions with parallel in- and out-currents in the x-direction are favored; those with anti-parallel currents are suppressed. There is no bias in the $\hat{y}$-direction. If $b = 0$ the LGA satisfies detailed balance and represents random walkers interacting through the Fermi exclusion rule. All spatial correlations are vanishing. If $b \neq 0$ there exists a spatially uniform equilibrium state with long range correlations $\sim 1/r^2$. The qualitative features of this model are similar to those of the diffusive lattice gas, studied in [8].

It is important to emphasize that the constraints of (semi)-detailed balance, i.e.

$$\begin{aligned} &\sum_s F_0(s) A_{s\sigma} = F_0(\sigma) && (SDB) \\ &F_0(s) A_{s\sigma} = F_0(\sigma) A_{\sigma s} && (DB) \end{aligned} \tag{4.3}$$

refer to the factorized Gibbs distribution $F_0(s) = C \exp[\alpha\rho(s) + \ldots]$, which depends on the state variable s only through the conserved densities $\rho(s)$, etc. This implies $F_0(s) = F_0(\sigma)$ and the SDB constraints reduce to the familiar form $\sum_s A_{s\sigma} = 1$. Similarly the DB constraints in (4.3) reduce to $A_{s\sigma} = A_{\sigma s}$.

Therefore the model properties $\sum_s A_{s\sigma} \neq 1$ or $A_{s\sigma} \neq A_{\sigma s}$ do exclude the existence of the Gibbsian equilibrium state, but do *not* necessarily imply the existence of position and velocity *correlations* in equilibrium. This statement can be slightly rephrased by saying that the model properties $\sum_s A_{s\sigma} \neq 1$ or

$A_{s\sigma} \neq A_{\sigma s}$ do *not exclude* the existence of a completely *factorized equilibrium* distribution. We present an example.

Consider a variation on the LGA in (4.2) of a driven diffusive system, where

$$A_{s\sigma} = \frac{1}{Z(s)} \delta(\rho(s), \rho(\sigma)) \exp[\boldsymbol{j}(\sigma) \cdot \boldsymbol{E}]. \tag{4.4}$$

Here $\boldsymbol{E}$ is an external bias field and $\boldsymbol{j}(s) = \sum_i \boldsymbol{c}_i s_i(r)$ the local (non-conserved) particle current. Then clearly, $\sum_s A_{s\sigma} \neq 1$. Nevertheless, the SDB- or DB-condition (4.3) does admit a completely factorized (normalized) equilibrium solution,

$$F_0(s) = C \exp[\alpha \rho(s) + \boldsymbol{j}(s) \cdot \boldsymbol{E}], \tag{4.5}$$

which can also be cast in the standard form (3.2) with an equilibrium single particle distribution of Fermi-type,

$$f_i = \left[1 + \exp(-\alpha - \boldsymbol{c}_i \cdot \boldsymbol{E})\right]^{-1}. \tag{4.6}$$

Establishing the stability of this equilibrium state (4.5)-(4.6) requires an H-theorem. In fact, at this meeting H. Chen [14] has presented a proof of the H-theorem for a lattice gas that satisfies the DB-condition (4.3) with respect to a factorized equilibrium distribution (4.5) with $\exp[-\boldsymbol{j}(s) \cdot \boldsymbol{E}]$ replaced by $\Pi_j (F_j / I_j)$, where F_j and I_j are arbitrary positive constants.

Concluding, we can say that the model satisfies the SDB-constraints (4.3) with respect to the *factorized* distribution $F_0(s)$. The source term B_{ij} in (3.10) vanishes for this model and consequently all on- and off-node correlations vanish in the equilibrium state.

5 Conclusion

We have studied LGA's with local (on-node) interactions that possess slow (diffusive or hydrodynamic) modes and lack (semi)-detailed balance (SDB) with respect to the Gibbs distribution. As is well known [1, 2, 8], for long times such systems approach non-thermodynamic spatially uniform states, which exhibit long range correlations, if the isotropic spatial symmetry is broken by externally applied fields or reservoirs. The surprising result is that there exist LGA's that exhibit long-range spatial correlations $\sim r^{-d-2}$

in the equilibrium state without any fields or reservoirs that break the spatial symmetry. These correlations are absent in LGA's satisfying (semi)-detailed balance. The property $\sum_s A_{s\sigma} \neq 1$, i.e. violation of the standard SDB-constraints, does not necessarily imply the existence of long range correlation, nor does it exclude the existence of a completely factorized equilibrium distribution. This was shown by explicit construction of a diffusive LGA model that satisfies the SDB-constraints with respect to a non-Gibbsian factorized equilibrium distribution (see (4.5) and (4.6)). A similar fluid-type LGA has been presented at this meeting by H. Chen [14]. In continuous fluids long-range correlations and non-detailed balance stationary states can only exist in open systems, externally driven or constrained by reservoirs, because the thermodynamic (Gibbs) equilibrium state satisfies detailed balance.

Acknowledgements

The authors wants to thank J.R. Dorfman and J.W. Dufty for stimulating discussions. H.J.B. acknowledges financial support by the "Stichting voor Fundamenteel Onderzoek der Materie" (FOM), which is sponsored by the "Nederlandse Organisatie voor Wetenschappelijk Onderzoek" (NWO).

References

[1] J.R. Dorfman, T.R. Kirkpatrick and J.V. Sengers, Ann. Rev. of Phys. Chem. 45, 213 (1994).

[2] M.Q. Zhang, J.S. Wang, J.L. Lebowitz and J.L. Valles, J. Stat. Phys. 52, 1461 (1988).

[3] G. Grinstein, D.-H. Lee and S. Sachdev, Phys. Rev. Lett. 64, 1927 (1990).

[4] G. Grinstein, J. Appl. Phys. 69, 5441 (1991).

[5] M.H. Ernst and E.D.G. Cohen, J. Stat. Phys. 25, 153 (1981).

[6] J.W. Dufty and M.H. Ernst, in: 'Pattern formation and lattice gas automata', (proceedings NATO workshop, Waterloo, Canada, June 7-12, 1993), A. Lawniczak and R. Kapral, eds., Fields Institute Communications (Am. Math. Soc.).

[7] H.J. Bussemaker, M.H. Ernst and J.W. Dufty, J. Stat. Phys. 78, 1521 (1995) [preprint: comp-gas@xyz.lanl.gov/9404002].

[8] Z. Cheng, P.L. Garrido, J.L. Lebowitz and J.L. Valles, Europhys. Lett. 14, 507 (1991).

[9] B. Dubrulle, U. Frisch, M. Hénon and J.-P. Rivet, J. Stat. Phys. 59, 1187 (1990).

[10] M. Hénon, J. Stat. Phys. 68 (1992) 409; M. Hénon, in: 'Pattern formation and lattice gas automata', (proceedings NATO workshop, Waterloo, Canada, June 7-12, 1993), A. Lawniczak and R. Kapral, eds., Fields Institute Communications (Am. Math. Soc.).

[11] H.J. Bussemaker and M.H. Ernst, J. Stat. Phys. 68, 431 (1992).

[12] B. Boghosian and W. Taylor, preprint comp-gas@xyz.lanl.gov/9403003; see also these proceedings.

[13] H.J. Bussemaker and M.H. Ernst, to be published.

[14] Hudong Chen, these proceedings.